Conductivity of disordered quantum lattice models at infinite temperature: Many-body localization

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We reinvestigate the behavior of the conductivity of several disordered quantum lattice models at infinite temperature using exact diagonalization. Contrary to the conclusion drawn in a recent investigation of similar quantities in identical systems, we find evidence of a localized regime for strong random fields. We estimate the location of the critical field for the many-body localization transition for the random-field XXZ spin chain, and compare our findings with recent investigations in related systems.

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I. INTRODUCTION

Anderson localization in non-interacting systems is a well understood physical process whereby sufficiently strong disorder leads to localization of eigenstates and hence insulating behavior in systems that would otherwise be conductors. Extensive work performed over the last 50 years has established in great detail the nature of the Anderson transition in non-interacting systems, while much less work has been aimed at elucidating how short-ranged interactions modify the simple picture of transport that emerges in the non-interacting situation. This is somewhat surprising, given the fact that attention to the issue of interactions already appears in Anderson's classic 1958 paper.

Recently Basko, Aleiner and Altshuler (BAA) performed a detailed diagrammatic analysis demonstrating that weak, short-ranged electron-electron interactions generically lead to a finite temperature metal-insulator transition in systems that would be localized in the absence of interactions.⁴ In fact the analysis and implications of the work of BAA go beyond consideration of interacting electrons, suggesting that more general quantum entities (e.g. spins, bosons) with local interactions may generically fail to thermalize until a threshold energy is reached. The notion that such a "many-body" localization (MBL) transition may occur is at odds with the intuition that interactions should lead to a finite dc conductivity at all finite temperatures in analogy with the mechanism of phonon-mediated hopping conductivity. It is also at odds with, for example, the analysis of Fleishman and Anderson which argues that truly short-ranged interactions are insufficient to induce conductivity in an otherwise localized system at any temperature.⁵

The work of BAA has motivated more recent investigations of the possibility of a finite temperature transition from a localized (non-ergodic) phase to a delocalized phase where interactions afford thermalization of the system. These works, both analytical and numerical, have reached somewhat conflicting conclusions. ^{6–10} In this work, we reconsider the analysis of Karahalios et al. ⁸ Via examination of the conductivity, these authors concluded that, in general, finite temperature systems of

one-dimensional interacting spins are always conducting, thus contradicting the claim of BAA.

II. IMAGINARY FREQUENCY CONDUCTIVITY

Here, as in previous work, we make use of the important observation of Oganesyan and Huse that the manybody localization transition may be probed at infinite temperature by varying the disorder strength. This simplifies the problem by reducing the number of control parameters that may be varied to tune the system from a delocalized to a localized phase. As in the work of Karahalios et al., we examine one-dimensional spin chains via exact diagonalization, calculating the conductivity via the Kubo formula. An important conclusion of our work is that sufficient care needs to be exercised in the interpretation of the zero frequency conductivity as a function of disorder strength and level broadening.

For a finite system of length L at $T \to \infty$, the Kubo formula for the conductivity is given by

$$\sigma(\omega) = \frac{\beta}{L} \lim_{\eta \to 0} \int_0^\infty e^{i(\omega + i\eta)t} \langle j(t)j(0)\rangle dt, \qquad (1)$$

where $\beta = 1/k_BT$, j(t) is the current operator at time t, and η can be thought of as both a numerical tool for convergence as well as a phenomenological level broadening for discrete spectra. The real part of the conductivity may be decomposed as $\sigma'(\omega) = D\delta(\omega) + \sigma_{\rm reg}(\omega)$, where the Drude weight D measures purely ballistic conduction and arises due to pairs of degenerate states connected by the current operator. However, in the systems studied here, all level degeneracies are lifted in the presence of disorder, and conductivity is purely diffusive. Thus we may take as our definition of the dc conductivity $\sigma_{\rm dc} = \sigma(\omega \to 0)$ without concern for the Drude contribution. By employing the spectral representation of the Hamiltonian we arrive at the 'imaginary frequency' dc conductivity.

$$\sigma(i\eta) = \frac{\beta}{ZL} \sum_{m,n} |\langle m|j|n\rangle|^2 \frac{\eta}{\eta^2 + (\omega_{nm})^2}, \qquad (2)$$

where $H|n\rangle = E_n|n\rangle$, $\omega_{nm} = E_n - E_m$, and Z is the partition function.

The authors of Ref.[8] calculate the full frequency-dependent (ac) conductivity spectrum using a level-broadening binning procedure and draw conclusions regarding dc conductivity based on the $\omega \to 0$ behavior. However, as we will show, all finite-sized systems with level broadening will exhibit a non-zero dc conductivity, and thus such an analysis is inconclusive. Rather, it is the conductivity's dependence on this level broadening which allows one to draw conclusions regarding conducting and insulating behaviors in the thermodynamic limit.

As discussed by Thouless and Kirkpatrick, ¹² finite systems should display a simple asymptotic behavior for the dc conductivity that scales as η for small η and η^{-1} for large η . The distinction between conductor and insulator manifests in the behavior between these asymptotic regimes. In particular, we expect that a system with insulating behavior will exhibit an imaginary frequency dc conductivity with well resolved η and η^{-1} regimes separated by a simple maximum. Finite sized systems expected to behave as conductors in the $L \to \infty$ limit exhibit a broad crossover between these regimes, with a plateau signifying the onset of a true dc conductivity. 11,12 Although the dc conductivity is well defined only in the thermodynamic limit (specifically, $L \to \infty$, then $\eta \to 0$), we see evidence for dc conductivity manifesting itself even at the small system sizes accessible by exact diagonalization.

It should be pointed out that although the analysis employed here was originally developed for non-interacting systems, our results empirically show that it is equally applicable to interacting ones, by replacing the single-particle levels with many-body levels. Specifically, we locate an insulating regime in which $\sigma(i\eta) \propto \eta$ when η is less than the level spacing in the many-body localization volume, which does not scale with the size of the system. This behavior is to be contrasted with an observed metallic regime, which has $\sigma(i\eta) \propto \eta$ as long as η is less than the many-body level spacing in the system volume – a spacing which vanishes in the thermodynamic limit yielding a dc conductivity plateau at small to intermediate η .

III. QUANTUM LATTICE MODELS

We study two quantum lattice models in the presence of disorder: the XXZ spin chain and the t-t'-V model of spinless fermions, originally studied in its disordered form by Oganesyan and Huse⁶ and more recently by Monthus and Garel.¹³ The disordered XXZ chain is given by the

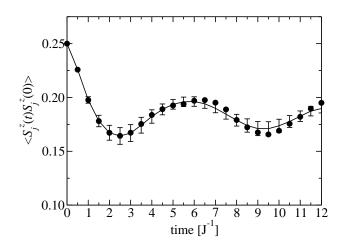


FIG. 1: Local spin-spin correlation function, $\langle S_{j}^{z}(t)S_{j}^{z}(0)\rangle$ for the disordered XXZ chain with W=5. Results are shown for the non-interacting case, $\Delta=0.0$ (filled circles) and for the interacting case, $\Delta=0.5$ (solid line). Error bars for the non-interacting case (not shown for clarity) are of the same order as those shown for the interacting case.

Hamiltonian

$$H_{XXZ} = J \sum_{j=1}^{L} \left[S_j^x S_{j+1}^x + S_j^y S_{j+1}^y + \Delta S_j^z S_{j+1}^z \right] + \sum_{j=1}^{L} w_j S_j^z,$$
(3)

where we choose the random fields w_j uniformly from [-W, W]. The current operator for the XXZ chain is given by

$$j_{XXZ} = J \sum_{j=1}^{L} \left[S_j^x S_{j+1}^y - S_j^y S_{j+1}^x \right]. \tag{4}$$

The disordered t-t'-V model is described by the Hamiltonian

$$H_{t-t'-V} = \sum_{j=1}^{L} \left[-t \left(c_{j}^{\dagger} c_{j+1} + c_{j+1}^{\dagger} c_{j} \right) - t' \left(c_{j}^{\dagger} c_{j+2} + c_{j+2}^{\dagger} c_{j} \right) + V \left(n_{j} - \frac{1}{2} \right) \left(n_{j+1} - \frac{1}{2} \right) + w_{j} n_{j} \right],$$
 (5)

where, following Oganesyan and Huse, the random onsite energies w_j are chosen from a Gaussian distribution with mean 0 and variance W^2 . The t-t'-V model's current operator is

$$j_{t-t'-V} = i \sum_{j=1}^{L} \left[t \left(c_j^{\dagger} c_{j+1} - c_{j+1}^{\dagger} c_j \right) + 2t' \left(c_j^{\dagger} c_{j+2} - c_{j+2}^{\dagger} c_j \right) \right].$$
 (6)

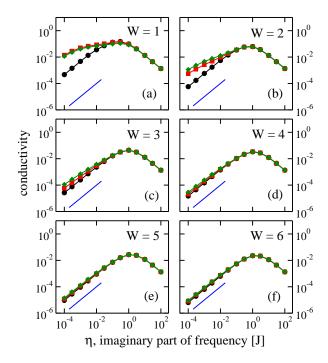


FIG. 2: The dc conductivity as a function of the imaginary frequency, η , for the disordered XXZ chain (J=1) with W=1-6 [(a)–(f)] for the non-interacting case, $\Delta=0.0$ (black line, circles) and for two interacting cases, $\Delta=0.5$ (red line, squares) and $\Delta=1.0$ (green line, diamonds). Error bars are smaller than the symbols. The blue line shows linear slope.

In what follows, we restrict our Hilbert space to $S^z_{tot}=0$ for the XXZ chain and to half-filling for the t-t'-Vmodel. We have explored other alternatives and find our results to be qualitatively similar. All results are presented for L = 14 with periodic boundary conditions, although we have studied systems as large as L = 16and find our conclusions unaltered. We average over $N_r = 100$ independent realizations of disorder and calculate error bars as the standard deviation of the mean, $\pm \sigma/\sqrt{N_r}$, where σ (not to be confused with the conductivity) is the standard deviation across disorder realizations. Our results appear to be converged, although for such a small range of system sizes one should view such statements with care. This is especially true for smaller values of disorder, where finite localization lengths, if they exist, can clearly be larger than the system sizes accessible from exact diagonalization.

The aforementioned claim of Karahalios et al. is rather surprising in light of the fact that an earlier tDMRG calculation performed on strongly disordered spin chains found evidence of a localized phase, at least when viewed from the standpoint of the local spin-spin correlation function. In Fig. 1 we reproduce this result (for a smaller system and the shorter time scales accessible in exact diagonalization) and compare it with dynamics in the non-interacting system which is known to be localized. It is clear that, for the interacting system, the local spin-

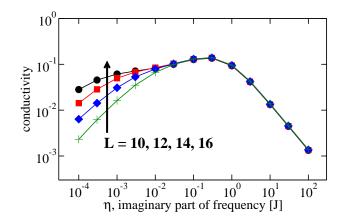


FIG. 3: System size dependence of the dc conductivity as a function of the imaginary frequency, η , for the disordered XXZ chain (J=1) with $\Delta=0.5$ and W=1. Conductivities are presented for L=10 (green plusses), 12 (blue diamonds), 14 (red squares), and 16 (black circles), showing the development of the dc conductivity plateau in the $L\to\infty$ limit.

spin correlation exhibits quantitatively similar relaxation compared to the localized system and shows no sign of decay from a plateau (the analog of the Edwards-Anderson parameter), indicative of a glassy phase.

IV. RESULTS AND THE MANY-BODY LOCALIZATION TRANSITION

We turn next to an investigation of the conductivity in the above disordered lattice models. As discussed above, it is useful to compare the η dependence of the dc conductivity in the interacting models directly with their noninteracting counterparts to set a baseline for localization. In Fig. 2 we present results for two different values of the anisotropy Δ in the XXZ spin chain. We extend the results of Karahalios et al., who examine disorder strengths only as high as W = 1, by performing our calculations up to W = 6. Clearly, by W = 4 in both interacting cases the conductivity curves are essentially indistinguishable from the non-interacting localized case. Thus, at least with regard to exact diagonalization on these system sizes and based solely on examination of the conductivity, the interacting behavior is identical to the non-interacting, localized behavior. Using this condition, we can place an upper limit, $W_c \lesssim 4$ in both cases $\Delta = 0.5$ and $\Delta = 1.0.17$ It should be noticed as well that already at W = 1 there is significant structure in $\sigma(i\eta)$, exhibiting a nearly flat region in between the small and large η regimes. This suggests that these interacting data are in a conducting regime, although care must be used because this also might be an indication of localization behavior on length scales larger than we can access via exact diagonalization. One should also note that this conducting behavior is fully consistent with the conclusions of Karahalios et al. at W = 1.0.

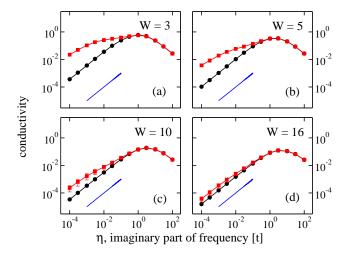


FIG. 4: The same as in Fig.2 but for the disordered t-t'-V model (t = t' = 1) with W = 3 (a), W = 5 (b), W = 10 (c), and W = 16 (d), for the non-interacting case, V = 0 (black line, circles) and for the interacting case, V = 2 (red line, squares). Where not shown, error bars are smaller than the symbols. The blue line shows linear slope.

With the above caveats, we can place the critical value of W for a many-body localization transition in the range $3 < W_c < 4.^{18}$ It is thus unsurprising that Karahalios et al. found no evidence for the MBL transition, as we have shown that it occurs at disorder strengths larger than those investigated in Ref.[8]. We have additionally analyzed adjacent many-body level-spacings (not shown here), whose crossover from the Gaussian Orthogonal Ensemble to Poisson statistics $^{14-16}$ occurs at this same critical strength of disorder, confirming the robustness of our approach.

In order to confirm our expectations of a conducting phase in the thermodynamic limit, $L \to \infty$, we have examined the effects of system size on the conductivity of the interacting XXZ spin chain with $\Delta = 0.5$. We focus on the disorder strength W=1 because of its apparent conducting behavior in Fig. 2. Furthermore, one is in danger of approaching localization lengths equal to the size of the sytem for values of disorder much smaller than this. We show in Fig. 3 the conductivities for system sizes $L=10,\,12,\,14,\,\mathrm{and}\,16.$ Results for L=16 are shown for $N_r = 50$ realizations of disorder. Clearly, the plateau becomes more resolved for larger system sizes, strongly suggesting a non-zero dc conductivity in the thermodynamic limit. Furthermore, the plateau's growth extends toward smaller η in agreement with the many-body level spacing discussion above.

We have also examined the behavior of the disordered t-t'-V model of Oganesyan and Huse, the results of which are presented in Fig. 4. The behavior is qualitatively the same as above, suggesting the existence of a MBL transition in this model as well. However, it should be pointed out that the crossover between apparent conducting and insulating behavior in $\sigma(i\eta)$ is significantly broader in the t-t'-V model than in the XXZ systems, making a prediction of the critical disorder strength difficult. At larger system sizes this crossover should become more abrupt, but unfortunately such sizes are beyond the reach of exact diagonalization. Despite the above difficulties, we would expect, based on the same means of analysis presented above, that the critical value of W in this model is higher than the $W_c \approx 5$ range found in the real-space renormalization group calculation of Monthus and Garel. Although, it is not clear when studying finite systems that different quantities, such as those investigated here and by Monthus and Garel, should behave in a similar manner. However, our result does strongly suggest conducting behavior at $W \approx 5$.

V. CONCLUSIONS

To summarize, we have carried out a systematic investigation of the diffusive conductivities of two common disordered quantum lattice models: the XXZ spin chain and the t-t'-V model of spinless fermions. We find that by studying the behavior of $\sigma(i\eta)$ we can place reasonable bounds on the location of the MBL transition. By examining disorder strengths higher than those explored in previous works, we find for the disordered XXZ chain (both $\Delta = 0.5$ and $\Delta = 1.0$) that the finite size conductivity extrapolates quantitatively to the non-interacting values by $W \approx 4$. Our results are also qualitatively consistent with the recent work of Monthus and Garel, but we would expect based on finite size studies of the conductivity, that the transition occurs at a disorder value larger than that found by their numerical renormalization group procedure.

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- It should be noted that it is possible that a residual conductivity, impossible to resolve via an exact diagonalization study of σ_{dc} on small systems, exists. We see no evidence for finite size effects here, though we are restricted to very small L.
- 18 After this work was completed we became aware of the work of Pal and Huse (arXiv:1003.2613v1), who also investigate the XXZ chain with $\Delta=1$. Their conclusions are quantitatively consistent with our results. It should be noted that their work goes beyond that presented here by connecting the MBL transition to the infinite randomness universality class.